

Fermi Gas*

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A theory is developed for magnetically confined Fermi gas at low temperature based on the density functional theory. The theory is illustrated by numerical calculation of density distributions of Fermi atoms ^{40}K with parameters according to DeMarco and Jin's experiment[Science, 285(1999)1703]. Our results are in good agreement with the experiment. To check the theory, we also performed calculations using our theory at high temperature and compared very well to the result of classical limit.

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In a recent publication, DeMarco and Jin reported their work on Fermi atoms at low temperature in confined geometries. They employed an evaporative cooling strategy to cool a magnetically trapped gas of 7×10^5 ^{40}K atoms to 0.5 of the Fermi temperature T_F . An Ioffe-Pritchard-type magnetic trap [2] provides a cylindrically symmetric, harmonic potential with an axial frequency of $\omega_z = 2\pi \times 19.5$ Hz and a variable radial frequency. The radial frequency, as well as the minimum magnetic field, can be smoothly varied from $\omega_r = 2\pi \times 44$ Hz to $2\pi \times 370$ Hz by changing the current in a pair of Helmholtz bias coils. In the experiment presented by DeMarco and Jin, a single-component gas of the $F = 9/2$, $m_F = 9/2$ atoms is produced, where F is the total atomic spin and m_F is its magnetic quantum number. The time-of-flight image was taken by suddenly switching off the current that provides the magnetic trapping field, which allowed the gas to expand freely for 15 to 20 ms. The absorption shadow, generated by illumination of the expanded gas, was imaged onto a charged-coupled device array. They detected the emergence of quantum degeneracy in a trapped gas of Fermionic atoms and observed a non-classical momentum distribution and found that the total energy of the gas is larger than the classical expectation. They observed not only the momentum distribution but also the confined gas itself, which approaches a fixed size as T approaches zero.

In this letter, we present a general theory of the low-temperature density profile of an ideal Fermi gas trapped within an arbitrary potential well. Then we give the results of numerical

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calculation to compare to the experiment. The approach taken here is based on the density functional theory (DFT) [4,5], which was first introduced by Kohn and Hohenberg [6] in the context of ground state energy of quantum systems. It was developed and extended to excited states and to finite temperatures by some researchers and has become the effective first principle calculational method for the electronic and structural properties of a large variety of condensed matter systems. Considering a single-component system within an external potential at $T \neq 0K$, the DFT asserts that the true density distribution of a system in an external field $V(\mathbf{r})$ is the one that leads to the minimum of the following functional,

$$F[n(\mathbf{r})] = F_0[n(\mathbf{r})] + \int [V(\mathbf{r}) - \mu] \cdot n(\mathbf{r}) d\mathbf{r}, \quad (1)$$

and the minimum is the the Helmholtz free energy of the system. Here μ is the chemical potential in the above expression. While $F_0[n(\mathbf{r})]$ is a temperature dependent functional of $n(\mathbf{r})$ only, the dependence of $F_0[n(\mathbf{r})]$ on external potential $V(\mathbf{r})$ is only through the dependence of $n(\mathbf{r})$ on $V(\mathbf{r})$. This is a very strong statement which means that if we know the functional form of $F_0[n(\mathbf{r})]$ we can get all the physical quantities of interest. For a given external potential, the functional derivative of $F[n(\mathbf{r})]$ with respect to $n(\mathbf{r})$ should equals to zero:

$$\frac{\delta F[n(\mathbf{r})]}{\delta n(\mathbf{r})} = 0. \quad (2)$$

This gives an equation for $n(\mathbf{r})$, and when $n(\mathbf{r})$ is obtained from the solution of Eq. (2), we substitute it back to (1) to get the free energy and other quantities can be obtained simply by differential. It is hard to get the functional form of $F_0[n(\mathbf{r})]$, various approximations are employed in practical calculations. One of the commonly used approximation is the local density approximation(LDA) which usually gives excellent results to real systems. We use here the LDA in our theory of confined Fermi systems. In this approximation the functional $F_0[n(\mathbf{r})]$ is assumed to be

$$F_0[n(\mathbf{r})] = \int d\mathbf{r} f_0(n(\mathbf{r})). \quad (3)$$

And we assume that the free energy density $f_0(n(\mathbf{r}))$ has also the same functional form as the free energy of an uniform system of density n , i.e, $f_0(n)$ is the Helmholtz free energy density of an uniform system with density n . Then we can obtain

$$\frac{\delta F[n(\mathbf{r})]}{\delta n(\mathbf{r})} = \frac{\partial f_0(n(\mathbf{r}))}{\partial n(\mathbf{r})} + [V(\mathbf{r}) - \mu]. \quad (4)$$

According to Eqs. (2) and (4), we have

$$\partial f_0(n)/\partial n = \mu - V(\mathbf{r}). \quad (5)$$

For the ideal Fermi gas, we know [3]

$$n = \frac{1}{\lambda^3} f_{3/2}(z), \quad (6)$$

and

$$f_0 = -\frac{kT}{\lambda^3} f_{5/2}(z) + n kT \log z, \quad (7)$$

here

$$f_{5/2}(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty dx \cdot x^2 \log(1 + ze^{-x^2}),$$

$$f_{3/2}(z) = z \frac{\partial}{\partial z} f_{5/2}(z),$$

where k is Boltzmann's constant, $\lambda = \sqrt{2\pi\hbar^2/mkT}$ the thermal wave length, $z = e^{\beta\mu_0}$ the fugacity, and μ_0 the chemical potential of the uniform system. So we get

$$\partial f_0(n)/\partial n = kT \log z. \quad (8)$$

The value of μ is determined from the normalization of $n(\mathbf{r}, \mu)$:

$$N = \int n(\mathbf{r}, \mu) d\mathbf{r} \quad (9)$$

where we have indicated the μ dependence of n which follows from Eq. (5). Once having determined μ from Eq. (9) we substitute it back into Eq. (6) to get $n(\mathbf{r})$. Oliva has developed an approximate form of the Helmholtz free energy of the uniform system for different regimes of density [7]. However, in our theory such an expression of f_0 with respect to n is not required.

Now we use the confining potential well, according to the experiment by DeMarco and Jin, to calculate the density distributions of Fermi atoms.

We consider a harmonic potential form

$$V(r, z) = \frac{1}{2}m\omega_r^2 r^2 + \frac{1}{2}m\omega_z^2 z^2$$

which is cylindrically symmetric, where the axial frequency $\omega_z = 2\pi \times 19.5\text{Hz}$ and the radial frequency $\omega_r = 2\pi \times 137\text{Hz}$. The potential is independent of the azimuth angle. We have used the parameters given by the experiment setup, which is $N = 7 \times 10^5$ and $T = T_F/2$, with $T_F = \hbar(6\omega_z\omega_r^2 N)^{1/3}/k$ [8,9]. The value of T_F is $0.6\mu K$ for a million atoms in the $\omega_r = 2\pi \times 137\text{Hz}$ trap.

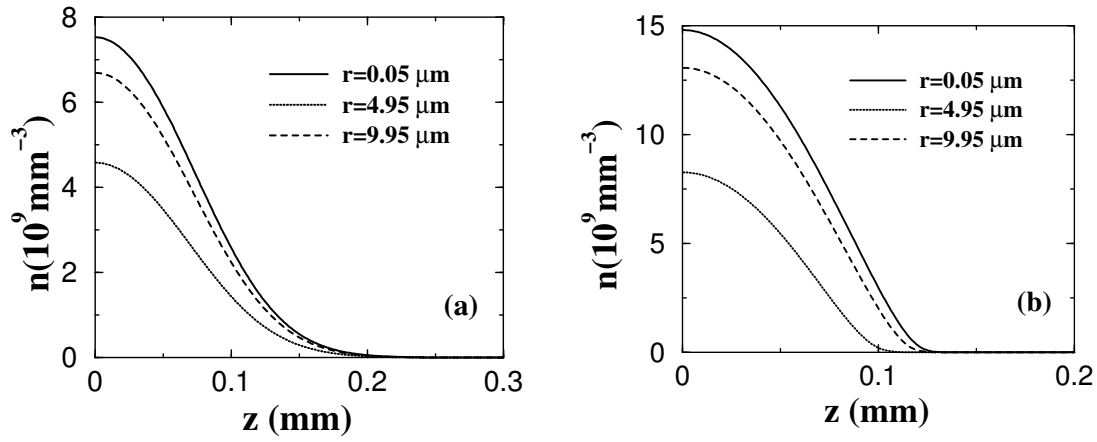


FIG. 1. Atomic density as function of z with different values of r for ^{40}K atoms under magnetic confinement. Total number of atoms $N = 7 \times 10^5$, (a) $T = 0.5T_F$, (b) $T = 0.05T_F$, with $T_F = 0.6\mu\text{K}$.

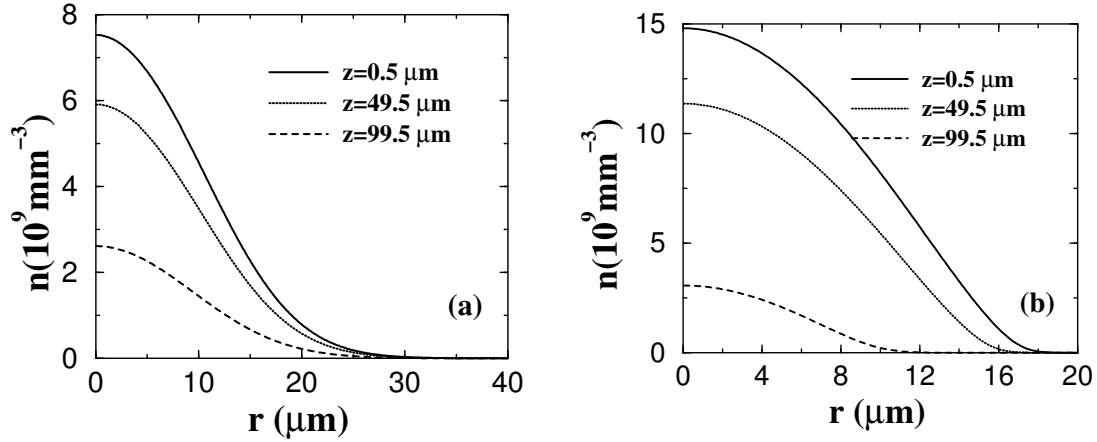


FIG. 2. Atomic density as function of r with different values of z for ^{40}K atoms under magnetic confinement. Other parameters are the same as Fig. 1.

The particle density distributions are calculated by using the present method. Figures 1 and 2 are plots of the density as function of z and r for two different temperatures. As observed in the experiment that the confined gas approaches a fixed size, we calculated the root-mean-square radius of the system and get $r_{RMS} = 0.7R_F$ at $T = 0.5T_F$ and $r_{RMS} = 0.5R_F$ at low temperature $T = 0.05T_F$, where $R_F = \sqrt{2kT_F/m\omega_r^2}$ [8,9]. These results are coincident with the experiment, where they obtained $r_{RMS} = 0.6R_F$ as T approaches zero and $r_{RMS} = 0.9R_F$ at $T/T_F = 0.5$ [1]. The difference between theory and experiment may due to the systematic uncertainty in T/T_F within the experiment. To check the validity of our method we calculated the case for $T/T_F = 2$ with other conditions unchanged. At high temperature (i.e., in the classical limit $T \gg T_F$), we have [8]:

$$\mu = -kT \log[6(\frac{T}{T_F})^3] \quad (10)$$

In our calculation the chemical potential of the system is $\mu = -5.86 \times 10^{-29}$ J at $T/T_F = 2$, while Eq. (10) gives -5.92×10^{-29} J, which is satisfactory. The comparison of density distributions of our theory with the classical statistics can be seen in Fig. 3.

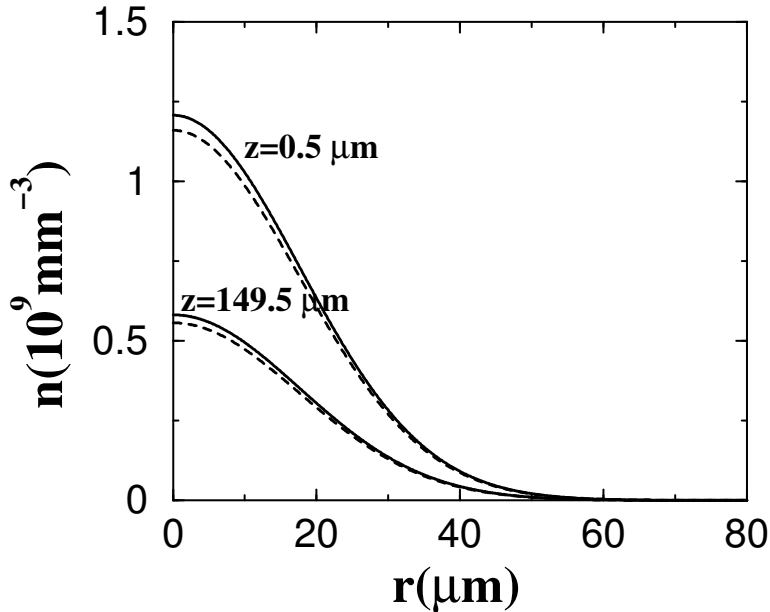


FIG. 3. Atomic density as function of r with different values of z for ^{40}K atoms under magnetic confinement. Parameters are the same as Fig. 1 except $T = 2T_F$. The solid lines are calculations from DFT as described in this work and dashed lines are from the Boltzmann distributions.

In summary we calculated the physical properties of the Fermi gas confined within a potential well at none-zero temperature. This method is based on the density functional theory under local density approximation. The case of ^{40}K atoms in a magnetic confinement is calculated and the result agrees with recent experiment. Here the interaction between atoms is completely neglected and the study of effect of interaction on the confined Fermi atomic gas is underway. Further studies of quantum degenerate Fermi gases in different confinement and interactions are also the important and interesting subjects.

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